



chain nodes :

1 2 3 4 10 11 12 13 14 20 21 22 23 24 27

ring nodes :

5 6 7 8 9 15 16 17

ring/chain nodes :

25

chain bonds :

1-2 1-11 2-3 2-10 3-4 3-5 9-12 12-13 12-14 14-15 15-20 20-21 20-22 21-23 23-24
23-25

ring bonds :

5-6 5-9 6-7 7-8 8-9 15-16 15-17 16-17

exact/norm bonds :

1-2 1-11 2-3 2-10 3-4 3-5 5-6 5-9 12-13 12-14 14-15 15-20 20-21 20-22 21-23
23-24 23-25

exact bonds :

6-7 7-8 8-9 9-12 15-16 15-17 16-17

isolated ring systems :

containing 5 : 15 :

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 27:CLASS 28:CLASS